DSSTox Field Definition File:

EPA High Production Volume (HPV) Challenge Program (HPVCSI)

Structure-Index File

(last updated 25 October 2007)

Description: Information in this file is intended to provide a minimum level of annotation to the DSSTox SDF (Structure Data Format) file created for the EPA High Production Volume (HPV) Challenge Program (HPVCSI) Chemical Lists. For further explanation of Source-specific fields and background pertaining to the content of this database, a user is encouraged to consult the Source Website below. Additional information is provided on the DSSTox HPVCSI SDF Download Page http://www.epa.gov/ncct/dsstox/sdf_hpvcsi.html. The DSSTox HPVCSI data file is an inventory of all chemical substances included in published EPA HPV Chemical Lists (http://www.epa.gov/chemrtk/pubs/update/hpvchmlt.htm). All HPVCSI Source fields and their entries and definitions were extracted from the Source Website listed below.

Description of ***DSSTox Standard Chemical Fields*** can be found in the Central Field Definition Table located at:
http://www.epa.gov/ncct/dsstox/CentralFieldDef.html

The HPVCSI Structure-Index data file contains no toxicity test data; hence, no ***DSSTox Standard Toxicity Fields*** are employed for this data file. Listed below are ***HPVCSI Source-Specific Fields*** containing chemical substance testing status information and URLs pointing to one of the 3 main EPA published lists of HPV Challenge chemicals (see Source Website). The ***Field Type*** indicates the type of the field, such as numeric, integer, defined text, memo, etc. All ***Units*** and ***Descriptions*** are extracted from Source reference materials unless otherwise noted. ***Allowable Entries*** lists allowed field entries occurring in HPVCSI, separated by slashes for exclusive entries (i.e., cannot occur with another entry) and semicolons or spaces for non-exclusive entries (i.e., can occur with other values). These are defined and explained in the ***Description*** section.

Source Website: EPA's High Production Volume (HPV) Challenge Program website http://www.epa.gov/hpv/.

SDF Usage Notes:
Each DSSTox SDF file contains a single **STRUCTURE** field. For each chemical record, the **STRUCTURE** field entry directly corresponds to the content of the **STRUCTURE_...** fields. The **STRUCTURE_Shown** field documents the relationship between what is displayed in the **STRUCTURE** field and the actual tested chemical substance, i.e. **TestSubstance_...** fields, with the latter corresponding directly to the toxicity data field entries. Commercial chemical relational database (CRD) applications may automatically insert one or more structure identifier fields upon import or export of an SDF file (e.g., Formula, FW or Mol_ID), fields that may augment or duplicate one or more of the DSSTox Standard Chemical Fields. Users are cautioned that fields containing null values in the first record of the SDF will be reordered upon import into most applications; for this reason, the word “blank” has been inserted into null fields in Record 1 of DSSTox SDF files and can be deleted after SDF import. Users are additionally cautioned that some fields (**STRUCTURE_SMILES** and **STRUCTURE_InChI**, in particular) may exceed the 200 character limit specified in the MDL CTFiles SDF standard (see http://www.epa.gov/ncct/dsstox/MoreonSDF.html), and that some CRD applications may insert a line break or truncate these fields upon SDF import or export. Finally, CRD application-specific molecular header information in the SDF file is deleted in the final DSSTox SDF files; users running CRD applications requiring a unique molecule header upon import of the SDF can specify either **DSSTox_RID** or the **DSSTox_FileID** be used. Upon SDF import, **DSSTox_CID** can be used to identify and manage chemical structure duplicates and **DSSTox_Generic_SID** can be used to identify common Test Substances across and within DSSTox files (similar to CASRN-substance, but available for all DSSTox substances and further distinguishes among different purity/grade substances).

As an MS Word document, the following table is best viewed onscreen using either Normal or Web Layout View in Landscape page orientation.

Field Name	***Field***	***Units***	***Allowable Entries***	***Description***	***Comments***

	Type				
HPVCSI Source-Specific Fields					
HPV_Indicator	defined text		0 (Within scope of HPV Challenge Program - may be sponsored); 1 (Not considered a candidate for testing); 2 (OECD HPV Information Screening Data Set - SIDS); 3 (Polymer or Inorganic); 4 (International Council of Chemical Associations - ICCA); 5 (No longer HPV)/	Entry signifies whether the chemical falls within or outside the scope of the HPV Challenge Program.	Values and expanded field entries were taken directly from the Source Website. *Field added to v2a.*
HPV_Chemical _Sponsorship_ Status ***(no spaces)***	defined text		Fully sponsored; ICCA confirmed commitment; Test Rule Chemical; Not sponsored; Provisionally Viable-Sponsored Chemical; Viable-Sponsored Chemical/	Entry signifies whether or not a chemical has been sponsored in the HPV Challenge Program, whether it is listed in the proposed "Testing of Certain High Production Volume Chemicals; Data Collection and Development on High Production Volume (HPV) Chemicals" rule (65 FR 81658), or whether it is listed in the Voluntary Children's Chemical Evaluation Program notice (64 FR 81699). ICCA = International Council of Chemical Associations	Field entries were taken directly from the Source Website. *Field added to v2a.*
HPV_TestPlan _Chemical ***(no spaces)***	defined text		Yes/ No/ *blank*	Test plan for chemical is available (Yes), will not be available (No), or status is indeterminant (*blank* or null entry).	Field entries were taken directly from the Source Website. *Field added to v2a.*
HPV_TestPlan_ ChemicalCategory *(no spaces)*	defined text		Acetic Acid & Salts/ Aliphatic Esters Category/ Alkaryl Sulfonate/ Alkenyl Succinic Anhydride/ ... *blank*	A chemical category, for the purposes of the HPV Challenge Program, is a group of chemicals whose physicochemical and toxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity. The large number of chemicals to be tested makes it important to reduce the number of tests to be conducted, where this is scientifically justifiable. One approach is to consider closely related chemicals as a group, or category, rather than test them as individual	Field entries were taken directly from the Source Website. *Field added to v2a.*

				chemicals. In the category approach, not every chemical needs to be tested for every SIDS (OECD HPV Information Screening Data Set) endpoint. However, the test data finally compiled for the category must prove adequate to support a screening-level hazard assessment of the category and its members. That is, the final data set must allow one to assess the untested endpoints, ideally by interpolation between and among the category members. In certain cases, such as where toxicity does not change among tested category members, extrapolation to the higher category members may be acceptable. See http://www.epa.gov/HPV/pubs/general/categuid.htm for more information. *blank* or null entry indicates an HPV Test Plan Chemical Category has not been assigned.	
Note_HPVCSI	memo		*text*	Field used to provide supplementary Source-specific information pertaining to the chemical and toxicity fields, with text entries to allow a user to easily locate added or modified records in version updates (see, e.g., CPDBAS)	
HPVProgram_ ChemicalList_URL *(no spaces)*	memo		*URL*	URL links to the EPA webpage providing description of the 3 main lists from which the current HPVCSI file was compiled: http://www.epa.gov/chemrtk/pubs/update/hpv_1990.htm ; http://www.epa.gov/chemrtk/pubs/update/hpv_1994.htm ; http://www.epa.gov/chemrtk/pubs/update/hpvadds.htm	The chemical substance content of HPVCSI is restricted to these 3 lists. A subset of this inventory with some additional substances has been incorporated into a related DSSTox file (HPVISD) corresponding to the on-line HPV Information System data collection. See: http://www.epa.gov/hpvis/. *Field was previously named* **Website_URL** *in v1a.*